

QDK/Chemistry: A Modular Toolkit for Quantum Chemistry Applications*

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Abstract

We present QDK/Chemistry, a software toolkit for quantum chemistry workflows targeting quantum computers. The toolkit addresses a key challenge in the field: while quantum algorithms for chemistry have matured considerably, the infrastructure connecting classical electronic structure calculations to quantum circuit execution remains fragmented. QDK/Chemistry provides this infrastructure through a modular architecture that separates data representations from computational methods, enabling researchers to compose workflows from interchangeable components. In addition to providing native implementations of targeted algorithms in the quantum-classical pipeline, the toolkit builds upon and integrates with widely used open-source quantum chemistry packages and quantum computing frameworks through a plugin system, allowing users to combine methods from different sources without modifying workflow logic. This paper describes the design philosophy, current capabilities, and role of QDK/Chemistry as a foundation for reproducible quantum chemistry experiments.

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1 Introduction

Quantum chemistry is among the most compelling application domains for quantum computers [1–4]. The promise of efficiently simulating strongly correlated electronic systems, where classical methods face exponential scaling, has motivated extensive algorithmic development over the past two decades [5–7]. Algorithms such as quantum phase estimation (QPE) [8–10] and variational quantum eigensolver (VQE) [11, 12] provide frameworks for extracting ground state energies and properties, while advances in error correction bring fault-tolerant implementations within reach [13, 14].

However, a quantum algorithm alone does not solve a chemistry problem. The path from a molecular structure to a meaningful energy estimate involves a substantial classical preprocessing pipeline: selecting a basis set, computing molecular integrals, performing mean-field calculations, choosing an active space that captures the essential correlation physics while conforming to hardware constraints, and mapping classical quantities (e.g., wavefunctions and Hamiltonians) onto qubit operators. These classical stages prepare inputs for quantum

execution which, much like classical computation, require extensive compilation and optimization to translate high-level algorithms into hardware-executable circuits. After quantum execution, classical postprocessing must aggregate measurement statistics into observable estimates. To connect with practical chemistry problems, multiple observable estimates need to be aggregated. Furthermore, in order to be comparable, all of the included calculations must have been computed in a consistent manner.

Consider, for example, a reaction energy profile. Computing this profile to obtain the reaction energy and barrier requires energy evaluations that include at least the starting, transition, and final states. Therefore, the solution of chemistry problems is not a single calculation, but rather a campaign executing multiple workflows, with each starting from structures with unique geometries and then proceeding through the aforementioned stages. Each of these stages involves methodological choices for the scientist, where the most optimal choice for each stage depends on the specific molecule, hardware platform, and scientific question at hand.

In practice, researchers often assemble these stages using *ad hoc* scripts that bridge multiple software packages. This approach often encounters several problems:

- Data formats differ between packages, requiring custom conversion code that is error-prone and rarely reusable.
- Methodological variations are difficult to track, hindering reproducibility.
- Comparing alternative approaches—i.e., different active space selectors, qubit mappings, or state preparation strategies—requires rewriting pipeline logic rather than simply swapping components.
- As quantum algorithms and hardware evolve rapidly, inflexible pipelines quickly become obsolete.

These challenges are not new [15–17] and not unique to quantum chemistry or quantum applications; similar issues arise across computational science domains where complex workflows span multiple software systems. The classical computational chemistry community has responded with modular frameworks for workflow management and interoperability, including workflow engines [18–22], standardized data schemas and archives [23, 24], plugin-based software architectures [25–27], and integrated platforms [28–30]. In parallel, the quantum computing community has developed frameworks specifically addressing the chemistry-to-circuit pipeline: OpenFermion [31] provides foundational data structures and fermion-to-qubit transformations; Tequila [32] offers high-level abstractions for variational algorithms with backend agnosticism; Tangelo [33] emphasizes end-to-end workflows with problem decomposition; and full-stack frameworks like Qiskit [34], PennyLane [35], and Cirq [36] provide circuit-level infrastructure with chemistry-specific extensions. These efforts have significantly advanced the field, yet each addresses a particular slice of the workflow: some focus on operator transformations, others on variational optimization, and still others on circuit compilation or hardware abstraction.

Despite a preponderance of successes, modular frameworks face a recurring tension: as they mature to address broader use cases, their abstractions often grow in complexity until significant expertise is required to understand, extend, or maintain them. The interfaces

designed to simplify component substitution can become barriers to entry when they accumulate layers of indirection. For quantum chemistry workflows targeting quantum computers, this tension is particularly acute because the field evolves rapidly—both the quantum algorithms and the classical methods that support them—and extensibility must remain practical rather than merely architectural.

With these considerations in mind, we have developed QDK/Chemistry¹: a permissively licensed, open-source, modular toolkit for the development and exploration of quantum chemistry workflows targeting quantum computers focusing on robustness, practical extensibility, and ease-of-use. The toolkit combines native implementations with capabilities from widely adopted open-source packages in the quantum chemistry and quantum computing communities, enabling researchers to leverage mature, community-tested software alongside purpose-built components. Rather than implementing a fixed pipeline, the toolkit defines interfaces that decouple workflow stages, enabling researchers to substitute methods at any stage without modifying surrounding code. This design serves the diverse needs of users across the quantum chemistry community:

- Application scientists can systematically explore methodological alternatives to determine which approaches work best for their molecules and scientific questions of interest.
- Method developers, ranging from classical electronic structure theorists to quantum algorithm developers, can integrate their implementations into a mature software stack without reconstructing the surrounding infrastructure.
- Educators and students gain access to a coherent framework for understanding the complete workflow from molecular specification to quantum measurement.

By serving the needs of these different user groups, QDK/Chemistry aims to accelerate progress toward practical quantum utility in the field of electronic structure calculations. Appendix A provides a complete code example demonstrating the workflow from molecular specification through quantum phase estimation.

QDK/Chemistry is an application library layer within the broader Microsoft Quantum Development Kit (QDK) [37], which provides the underlying infrastructure for quantum algorithm development and execution. The QDK encompasses the Q#, Qiskit, Cirq, and QASM programming languages for expressing quantum algorithms, compilers that translate high-level programs into optimized circuits, high-performance simulators for algorithm validation and debugging, and integrated development tooling within Visual Studio Code [38]. QDK/Chemistry builds on this foundation, leveraging QDK’s compilation and simulation infrastructure while providing the domain-specific data structures, algorithms, and workflows needed for quantum chemistry applications. Through its plugin architecture, the toolkit also integrates with the broader quantum software ecosystem, enabling researchers to combine QDK capabilities with external tools as their workflows require. This layered design allows chemistry researchers to focus on scientific questions while benefiting from ongoing advances in both the underlying QDK stack and the wider community of quantum chemistry and quantum computing software. The remainder of this paper discusses the design and software infrastructure underlying QDK/Chemistry, describes its current capabilities, and

¹<https://github.com/microsoft/qdk-chemistry>

outlines its role in the broader ecosystem of quantum chemistry and quantum applications software.

2 Software Design

The design of QDK/Chemistry reflects several principles that emerged from experience building quantum chemistry workflows for quantum computers. These principles guide architectural decisions throughout the codebase.

2.1 Separation of data and algorithms

A quantum chemistry workflow produces a sequence of intermediate results: a molecular geometry becomes a set of orbitals, which become a Hamiltonian, which becomes a qubit operator, and so on. In many codebases, these quantities are intertwined with the methods that produce them, making it difficult to substitute one method for another or to inspect intermediate results. QDK/Chemistry enforces a strict separation:

- Data classes represent intermediate quantities as immutable, self-contained objects.
- Algorithm classes are stateless transformations that consume data objects and produce new ones.

This separation yields a simple dataflow model: each stage takes well-defined inputs and produces well-defined outputs. Changing the method at one stage does not affect the behaviors at other stages (see Listing A for a concrete illustration).

Immutability of data classes, while seemingly restrictive, simplifies provenance: the output of a calculation depends only on its inputs and configuration, not on hidden state accumulated from previous operations. Algorithm configuration (e.g., method-specific options such as convergence thresholds, iteration limits) follows a similar pattern. Each algorithm exposes a type-safe settings object with easily discoverable parameters that locks after execution, preventing accidental modification. Both data and settings objects support serialization, enabling checkpointing and ensuring that calculations can be reproduced from archived inputs, and allowing for integrations with database and workflow management systems.

2.2 Uniform interfaces for algorithm substitution

Many workflow stages admit multiple implementations. Self-consistent field (SCF) calculations can use different convergence algorithms or different software backends; orbital localization can use different cost functions or proceed by different optimization strategies; qubit mapping can use different encodings with various trade-offs targeting different hardware; *et cetera*. In an ever-evolving landscape of methods, algorithms, hardware, and software, users should be able to switch implementations without rewriting pipeline code. This flexibility matters because different users have different goals: some are primarily interested in developing new algorithms, while others want to benchmark existing methods against their own problems of choice.

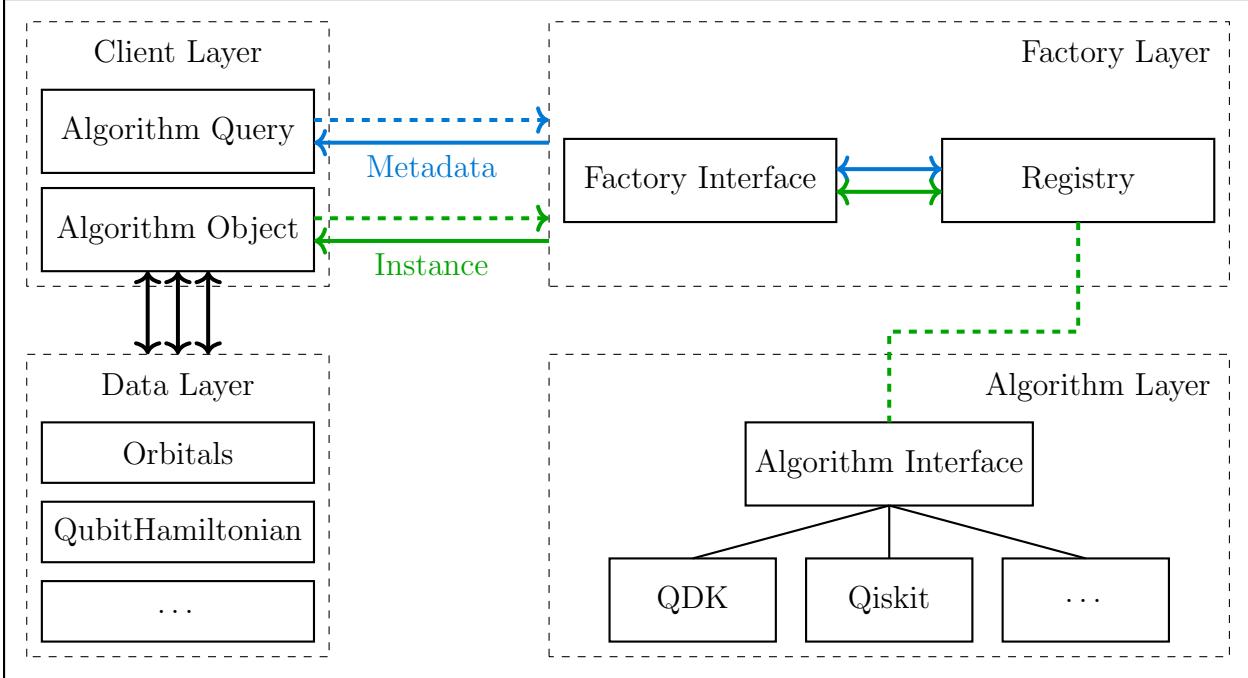


Figure 1: Architecture of QDK/Chemistry, illustrating the separation of client code, algorithm interfaces, factory registries, and data representations.

QDK/Chemistry achieves this through factory-based instantiation for algorithm interfaces. Each algorithm type has an associated factory that maintains a registry of available implementations. Conceptually, an algorithm interface is simply a name for all algorithms that require the same input data and produce the same output data. Users request an implementation by name; the factory returns an object conforming to the common interface. Client code operates on interfaces rather than concrete types, so substitution is transparent.

This pattern also supports discoverability. Users can query a factory at runtime to list available implementations, facilitating the exploration of alternatives. New implementations, whether developed internally or contributed by the community, integrate seamlessly once registered with the appropriate factory. Figure 1 illustrates the overall architecture of QDK/Chemistry, highlighting the separation of client code, algorithm interfaces, factory registries, and data representations.

2.3 Extensibility through plugins

No single codebase can implement every method of interest. Quantum chemistry has a rich ecosystem of specialized packages, and quantum computing frameworks continue to proliferate. A useful toolkit must integrate with this ecosystem rather than stand apart from it. Moreover, as quantum algorithms for chemistry evolve rapidly on both the hardware and algorithmic fronts, extensibility is essential for meeting current and future needs.

The plugin system in QDK/Chemistry is a foundational design choice rather than an afterthought. Treating extensibility as a first-class concern has become increasingly common in computational chemistry software, with major packages and workflow systems adopting

modular or plugin-based architectures [15, 16, 19, 20, 26, 27, 39, 40]. In the quantum applications domain, similar extensibility patterns appear [31, 33, 34, 41]. In QDK/Chemistry, plugins interact with the core exclusively through the same public interfaces available to any user, with no privileged access to internal state or implementation details. This minimal coupling ensures that plugins can be developed, tested, and maintained independently of the core codebase and of each other, maximizing reuse potential and reducing the maintenance burden as both the toolkit and its extensions evolve.

QDK/Chemistry uses a plugin architecture that supports two extension mechanisms. Developers can add new implementations of existing algorithm types, enabling integration with external packages. They can also define entirely new algorithm types with their own data contracts and factories, extending the workflow model itself. This capability is distinct from merely extending an existing interface.

Once registered, plugin implementations appear in factory registries alongside native implementations and are discoverable at runtime. Users need not distinguish between native and plugin-provided methods; the interface is uniform. This symmetry is intentional: a plugin-provided algorithm is a first-class citizen, indistinguishable in use from a native implementation, yet developed and maintained without dependence on the internals of the core or other plugins. This design allows QDK/Chemistry to serve as a coordination layer for heterogeneous tools while preserving the independence of each component.

Alongside this plugin-based extensibility, QDK/Chemistry includes robust, optimized native implementations for core workflow stages. These implementations coexist in the same factory registries as plugin-provided methods, giving users flexibility to choose based on their needs: whether leveraging familiar external tools or using purpose-built implementations tuned for the toolkit’s data structures. The plugin architecture and native implementations are complementary. Plugins extend the toolkit’s reach into the broader ecosystem, while native implementations offer tightly integrated alternatives that have been developed and tested alongside the core infrastructure.

An important consequence of this architecture is its compatibility with commercial and proprietary software. While the QDK/Chemistry framework itself is permissively licensed and open source, the plugin infrastructure imposes no licensing requirements on extensions. Plugins communicate with the core exclusively through public interfaces, without exposing implementation details in either direction. This separation enables collaborators to develop plugins that wrap proprietary codes, protecting intellectual property and respecting licensing constraints. Unlike “push-in” extensibility models that require contributions to reside within the main codebase, QDK/Chemistry plugins can be maintained in separate repositories under whatever access controls their developers choose. This design broadens the range of methods accessible through a unified interface, benefiting users who gain access to capabilities that might otherwise remain siloed.

2.4 Multi-language support

Quantum chemistry practitioners work in diverse environments: high-performance computing workflows often require compiled languages for efficiency, while rapid prototyping and interactive exploration favor Python. QDK/Chemistry addresses both contexts through a hybrid architecture: core data structures and algorithms are implemented in C++ for perfor-

mance, with Python bindings exposing identical application programming interface (API) through `pybind11` [42]. This approach follows successful precedents in packages such as PySCF [39] and Psi4 [40], which demonstrated that compiled computational kernels with Python-driven workflows can serve both high-performance and interactive use cases effectively. Users can develop workflows in whichever language suits their context, and mixed-language pipelines are straightforward.

This design also accommodates diverse developer preferences and the broader ecosystem of compiled codes. Researchers comfortable with Python can prototype new algorithms without learning C++, while performance-focused developers can work directly with the native implementation; both contribute through compatible interfaces. Beyond C++ and Python, QDK/Chemistry provides a consistent application binary interface (ABI) at plugin boundaries, enabling integration with external libraries written in C, Fortran, Rust, or other compiled languages through foreign function interfaces. This approach meets developers where they are, rather than where a particular toolkit might expect them to be, and enables integration with binary-distributed libraries when source access is unavailable or impractical.

Multi-language support extends to quantum circuit specification as well. Through the QDK, QDK/Chemistry can target quantum algorithms expressed in Q#, Cirq, Qiskit, and OpenQASM, allowing researchers to work in whichever quantum programming framework best suits their expertise or hardware requirements. This flexibility ensures that users are not locked into a single quantum ecosystem and can leverage advances in any of these rapidly evolving frameworks.

3 Capabilities

QDK/Chemistry supports the stages of a typical quantum chemistry workflow, from molecular specification through observable estimation. This section provides an overview of current capabilities; detailed documentation is available separately. Figure 2 illustrates the workflow stages, and Appendix A provides a complete code example.

3.1 Classical electronic structure

Classical electronic structure methods provide the foundation for quantum chemistry workflows, generating the molecular orbitals, reference wavefunctions, and correlation treatments that serve as inputs for quantum algorithms.

3.1.1 Molecular geometry handling

Typical quantum applications workflows begin with molecular geometry specification, which provides the atomic coordinates defining the system of interest. QDK/Chemistry manages molecular geometries through the `Structure` class, which represents atomic coordinates as immutable, self-contained objects. Currently, QDK/Chemistry requires geometries to be provided as input; geometry optimization capabilities are planned for future releases. Users can employ external packages for structure generation, e.g. geometry optimization, molecular dynamics, or experimental measurements, and import the resulting structures into

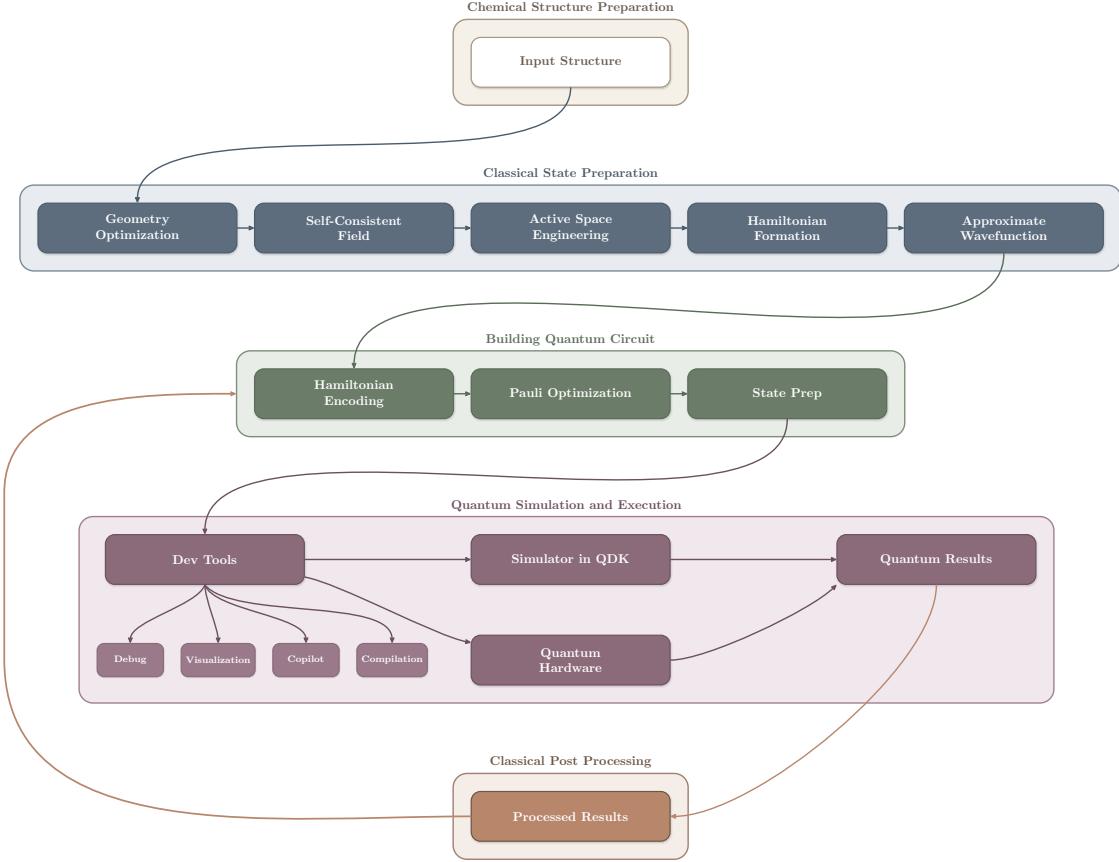


Figure 2: An example workflow orchestrated using QDK/Chemistry, from molecular geometry specification through to observable estimation.

QDK/Chemistry for subsequent stages. QDK/Chemistry accepts geometries in standard formats including XYZ files [43], as well as toolkit-provided schemas for text (JSON) and binary (HDF5) serializations. Molecular geometries arise from diverse sources—geometry optimization, reaction pathway sampling, molecular dynamics, experimental measurements, or manual construction—and QDK/Chemistry accepts these geometries without prescribing their origin. This design reflects the principle that structure generation is best handled by specialized tools, allowing users to employ their preferred methods for geometry preparation while leveraging QDK/Chemistry for quantum chemistry workflow stages. In larger pipelines, such as reaction network exploration but also molecular dynamics analysis, QDK/Chemistry is intended as a final stage to generate the most accurate wavefunction and properties for important sampled structures. This includes the analysis of a larger portion of sampled structures to determine their relevance by filtering based on energy criteria with e.g., density functional theory (DFT) and the analysis of optimal active space sizes to decide if calculations require a quantum computer.

3.1.2 Self-consistent field calculations

Mean-field SCF calculations produce initial wavefunctions and reference energies that anchor subsequent correlation treatments. The native SCF solver implements the geometric direct minimization algorithm [44], which frames orbital optimization as energy minimization on a Grassmann manifold rather than iterative diagonalization. This formulation provides robust convergence for systems where conventional diagonalization-based approaches struggle, including open-shell configurations, small-gap molecules, and transition metal complexes—precisely the systems where quantum algorithms are expected to provide the most significant improvements over classical methods [5–7]. Both Hartree-Fock (HF) and DFT methods are supported, with restricted, unrestricted, and restricted open-shell variants available for each. The native implementation builds on established libraries: Libint [45] for molecular integrals, Libcpint [46, 47] for effective core potential integrals, GauXC [48–51] for numerical integration on atom-centered grids, and Libxc [52] for exchange-correlation functional evaluation. In addition, the PySCF [39] plugin provides access to its comprehensive suite of electronic structure methods through the uniform QDK/Chemistry interface, enabling users to leverage this familiar tool within the modular framework.

Challenging SCF problems frequently converge to saddle points rather than true minima, producing reference states that compromise the quality of subsequent many-body calculations. QDK/Chemistry provides stability analysis tools [53] to detect these problematic solutions by examining the Hessian of the energy with respect to orbital rotations. When an instability is identified, users can perturb the wavefunction along the unstable mode and reoptimize using any implementation of the self-consistent field solver. This modular approach—separating stability detection from reoptimization—allows users to inspect intermediate results, apply domain-specific adjustments, and combine stability analysis with other orbital manipulation techniques as their workflow requires.

3.1.3 Orbital localization

Orbital localization transforms delocalized canonical orbitals into more compact representations that improve chemical interpretability, accelerate correlation method convergence, and facilitate active space selection. Canonical orbitals from SCF calculations are typically delocalized across the entire molecule, which can obscure chemical interpretation and slow the convergence of post-mean-field correlation methods. QDK/Chemistry provides several classes of orbital transformation techniques to yield representations that are “localized” in various senses: spatially compact, ordered by correlation importance, or partitioned by entanglement character. Each of these localization behaviors is beneficial for different downstream applications.

Spatial localization methods produce orbitals concentrated on bonds, lone pairs, or atomic sites by iteratively optimizing a cost function. QDK/Chemistry supports several established approaches through native implementations and plugin integrations, including through PySCF [39]: Pipek–Mezey [54] localization (minimizing orbital spread via Mulliken populations), Foster–Boys [55] localization (minimizing orbital second moments), and Edmiston–Ruedenberg [56] localization (maximizing self-repulsion integrals), each yielding orbitals with distinct characteristics [57–60].

Beyond spatial localization, orbital transformations can organize orbitals by correlation character. Natural orbitals [61], obtained by diagonalizing the one-particle reduced density matrix, order orbitals by occupation number; fractional occupations indicate significant correlation effects. QDK/Chemistry provides a native implementation of second-order Møller-Plesset perturbation theory (MP2) natural orbitals [62, 63], offering an efficient route to correlation-ordered orbitals without full multi-configuration calculations. This perspective complements spatial localization: spatially localized orbitals aid chemical interpretation and basis truncation, while natural orbital ordering guides active space selection and quantum resource allocation.

Localization in near-complete basis sets is numerically ill-posed for most iterative methods. QDK/Chemistry addresses this through the valence-virtual/hard-virtual separation [64, 65], partitioning virtual orbitals into chemically relevant and numerically problematic subspaces. This yields orbitals that vary smoothly with molecular geometry, which is valuable for consistent active space selection along reaction coordinates.

3.1.4 Active space selection

Active space selection identifies the subset of molecular orbitals that exhibit significant correlation effects and must be treated explicitly on the quantum computer, while freezing the remaining orbitals into classical contributions. Reducing quantum resource requirements is essential for early fault-tolerant quantum computers, and active space selection is among the most effective strategies for achieving this reduction. The challenge for active space selection is identifying which molecular orbitals exhibit significant correlation character and must be treated explicitly, while freezing the remaining orbitals into effective core and virtual subspaces that contribute only classically. An optimal active space should capture the essential many-body physics while remaining compact enough to fit within hardware qubit and gate budgets.

QDK/Chemistry provides both automated and manual approaches to active space selection. Entropy-based methods leverage concepts from quantum information theory to automatically identify strongly correlated orbitals based on their entanglement with the rest of the system [66–69]. A native implementation of the autoCAS algorithm [70, 71] computes single-orbital entropies from the one- and two-electron reduced density matrices of a multi-configurational wavefunction. Orbitals with high entropy—indicating strong entanglement with the remainder of the system—are included in the active space, while weakly entangled orbitals are frozen. The implementation includes both standard autoCAS and an enhanced variant (autoCAS-EOS) for improved robustness in challenging cases [72].

Occupation-based methods provide automatic selection using natural orbital occupation numbers from correlated many-body methods. Orbitals with fractional occupations indicate incomplete filling and associated correlation effects, warranting inclusion in the active space [63, 73, 74]. The atomic valence active space (AVAS) [75] method, available through the PySCF plugin, projects molecular orbitals onto a target atomic orbital basis—for example, metal 3d orbitals—to systematically identify valence active spaces appropriate for transition metal chemistry.

Valence-based selection offers a simpler approach, specifying active electrons and orbitals centered around the Fermi level based on chemical intuition about frontier orbital import-

tance. Beyond these structured approaches, QDK/Chemistry supports fully manual active space specification by directly populating the active space data within orbital objects. This capability enables expert users with domain-specific knowledge or superior chemical intuition to inject custom orbital partitionings that may not arise from automated selection criteria, ensuring that the toolkit accommodates both routine applications and specialized research workflows.

3.1.5 Multi-configuration wavefunctions

With an active space Hamiltonian constructed, multi-configuration (MC) calculations produce wavefunctions that capture correlation effects beyond the single-determinant mean-field approximation. While these methods provide more accurate energy estimates than SCF calculations, their primary role in quantum application workflows is twofold: generating high-quality initial states for quantum algorithms, and providing classical baselines against which quantum results can be compared. On scaled fault-tolerant quantum computers, classically computed MC wavefunctions serve as the foundation for state preparation circuits, enabling algorithms such as quantum phase estimation to target chemical accuracy for systems where classical methods face fundamental scaling limitations.

QDK/Chemistry supports two main classes of MC methods: orbital-frozen configuration interaction methods and orbital-optimized multi-configuration self-consistent field (MCSCF) methods. Both native complete active space configuration interaction (CASCI)/full configuration interaction (FCI) solvers and access to the comprehensive complete active space (CAS) capabilities of PySCF [39] are available through the uniform QDK/Chemistry interface, providing users with multiple options for classical active space correlation treatments. CASCI calculates an exact solution within the defined active space, with core orbitals frozen and virtual orbitals excluded [76]. However, the exponential scaling of exact diagonalization limits CASCI to modest active spaces.

Selected configuration interaction methods approximate the exact solution by iteratively identifying and including only the most important configurations, enabling treatment of substantially larger active spaces at the cost of controlled approximation [77–80]. QDK/Chemistry employs the adaptive sampling configuration interaction (ASCI) variant [81, 82] through native integration with Many-body Adaptive Configuration Interaction Solver (MACIS) [83], a high-performance selected configuration library for large-scale calculations. ASCI iteratively grows the determinant space by identifying configurations with the largest contributions to the wavefunction, achieving near-CASCI accuracy at a fraction of the computational cost and enabling treatment of active spaces that would otherwise be intractable. For users who prefer alternative multi-configuration implementations or require additional correlation treatments, the PySCF [39] plugin provides access to its wide range of multi-configuration and correlation methods through the same uniform interface.

The MC methods described in this section are entirely classical—they execute on conventional hardware and produce deterministic outputs including wavefunction coefficients and reduced density matrices. In this sense, classical CASCI and quantum CASCI solvers address the same underlying problem but differ in execution model and output contracts. As illustrated in Figure 2, the “Classical State Preparation” phase encompasses these classical correlation methods, while the subsequent “Building Quantum Circuit” and “Quantum Sim-

ulation and Execution” phases represent the transition to quantum computation. Within QDK/Chemistry, quantum algorithms serve as an alternative means of solving the active space problem—one that may ultimately scale to system sizes intractable for classical methods, but differ fundamentally in the nature of their outputs and execution requirements. We discuss quantum algorithms for energy estimation in Sections 3.2.3 and 3.2.4.

3.2 Quantum circuit construction

Quantum circuit construction transforms classical electronic structure data into executable quantum programs, encompassing the encoding of molecular Hamiltonians onto qubits, preparation of initial quantum states, and extraction of observable estimates through measurement.

3.2.1 Qubit Hamiltonian construction

Qubit Hamiltonian construction transforms fermionic molecular Hamiltonians into qubit operator representations suitable for quantum computation, encoding the electronic structure problem in a form that quantum hardware can process. Classical quantum chemistry methods express electronic interactions using second quantization, with fermionic creation and annihilation operators describing electron interactions. Quantum computers operate on qubits, necessitating a transformation from fermionic operators to qubit operators that preserves the anti-commutation relations essential to fermionic statistics. Standard fermion-to-qubit mappings include the Jordan–Wigner [84], Bravyi–Kitaev [85], and parity [86] transformations, each offering different trade-offs in operator weight and qubit connectivity requirements. More recent developments have produced mappings optimized for particular hardware topologies or molecular symmetries [87–91].

QDK/Chemistry implements the standard fermion-to-qubit transformations, representing the resulting qubit Hamiltonian as a sum of Pauli strings with associated coefficients. Custom encodings, including hardware-aware and system-adapted mappings, can be integrated through the plugin system.

3.2.2 State preparation

Quantum algorithms for chemistry require preparing quantum states that approximate the ground or excited states of molecular systems. In QDK/Chemistry, state preparation is viewed as a mapping between a classical representation of the molecular wavefunction—a Slater determinant or linear combination thereof, represented by the `Wavefunction` class—and a quantum circuit that prepares the corresponding state on a quantum computer given a particular qubit encoding.

This mapping can be accomplished through various techniques, including isometry encoding [92] for general states and linear combinations of unitaries for structured preparations [93–99]. However, when wavefunctions are sparse—containing few configurations with significant amplitudes—generic methods can be inefficient. QDK/Chemistry provides a specialized method for sparse wavefunction state preparation based on sparse isometries [100, 101], which avoid the exponential scaling associated with generic methods.

State preparation in QDK/Chemistry is modular and decoupled from the choice of downstream quantum algorithm. Users can inject their own state preparation circuits without modifying any other part of the workflow. The same state preparation circuit can feed into statistical energy estimation, quantum phase estimation, or other downstream algorithms, with the choice of preparation method orthogonal to the choice of observable extraction strategy. This separation reflects a practical reality: optimal state preparation depends on both the molecular system and the available quantum resources, and researchers developing novel preparation techniques benefit from the ability to integrate their methods into a complete workflow without reconstructing the surrounding infrastructure.

3.2.3 Statistical energy estimation

One approach to estimating observable expectation values, such as ground state energies, is through statistical sampling of measurements performed on prepared quantum states. This approach forms the foundation of VQE algorithms [11, 12, 102], where energy estimates guide classical optimization of parameterized quantum circuits. More broadly, statistical sampling applies whenever information must be extracted from quantum states, whether for variational optimization, benchmarking prepared states against classical references, validating quantum algorithm outputs, or reconstructing quantum states through tomographic techniques [103–106]. QDK/Chemistry supports this post-processing procedure through native implementations and plugin integrations.

This procedure begins by decomposing an operator of interest into a set of measurable components. For example, starting from a qubit-mapped Hamiltonian, represented as a linear combination of Pauli strings, terms can be grouped into sets of mutually commuting operators that share measurement bases, reducing the number of distinct circuit executions required [107–109]. QDK/Chemistry provides qubit-wise commutativity grouping through its Qiskit [34] plugin, enabling efficient batching of measurements and access to Qiskit’s circuit construction and transpilation capabilities. Additional optimizations filter Pauli terms with negligible expectation values given the prepared state, pre-computing their classical contributions rather than consuming quantum resources.

Measurement circuits execute on quantum hardware or simulators to obtain statistical samples for each operator group. Classical post-processing aggregates these measurement outcomes, combining statistics from each group with their corresponding Hamiltonian coefficients and pre-computed classical contributions to yield energy estimates. The statistical nature of quantum measurements introduces variance that decreases with increasing shot count, and QDK/Chemistry provides utilities for reassembling these measurements into final expectation values with uncertainty quantification (e.g., variance estimation).

3.2.4 Quantum phase estimation

While statistical energy estimation provides a practical approach for near-term devices, QPE offers a fundamentally different paradigm for extracting eigenvalues from quantum systems [8, 110, 111]. In the context of active space methods, QPE can be viewed as a quantum CASCI solver: it targets the same electronic structure problem within the defined active space, but executes on quantum hardware rather than classical processors. The core

structure of QPE consists of controlled unitary operations applied to a trial state, followed by an inverse quantum Fourier transform that extracts the encoded spectral information into a computational basis measurement. This modular structure naturally decomposes into independent components: state preparation, controlled unitary implementation, and phase readout.

The design space for each component admits significant variation. State preparation techniques range from simple product states to sophisticated multi-configuration ansätze. Controlled unitary implementation—the computational core of QPE—encompasses multiple paradigms: product formula approaches such as Suzuki-Trotter decomposition [112] approximate time evolution through sequences of simpler exponentials, while block encoding techniques [95, 96, 113, 114] embed the Hamiltonian into a larger unitary matrix, enabling quantum signal processing and qubitization methods with improved asymptotic scaling. Phase readout variants include standard QPE [110, 111] using multiple ancilla qubits for parallel phase extraction, and iterative approaches [115] that trade parallelism for reduced qubit overhead through sequential single-ancilla measurements. These algorithmic choices interact with hardware constraints: statistical estimation tolerates shorter coherence times suitable for near-term devices, while QPE achieves precision through circuit depth rather than shot count, becoming advantageous when hardware can sustain the required coherent evolution [94, 115–118].

The QDK/Chemistry implementation of QPE exemplifies the toolkit’s modular composability, factoring the algorithm into distinct layers that mirror this design space. The unitary construction layer currently provides product formula decompositions, with the interface designed to accommodate block encoding implementations as they become available through native development or plugin contributions. The mapper layer synthesizes constructed operators into controlled unitary circuits, while the phase extraction layer supports both standard and iterative readout variants. Each layer exposes its own algorithm interface through the standard factory-based extensibility mechanism, enabling researchers to contribute novel techniques—whether improved Hamiltonian simulation methods, optimized circuit synthesis strategies, or alternative phase extraction protocols—while relying on validated implementations elsewhere.

QPE execution uses the component specifications as input parameters that are composed internally into the complete circuit. This design enables transparent testing of algorithmic innovations: a new technique can be validated using QDK- or Qiskit-derived simulators before deployment to hardware providers, with the same specification producing identical circuit structure regardless of backend. For quantum circuit construction and execution, QDK/Chemistry offers parallel pathways through different backend ecosystems. The QDK [37] integration provides access to Q#-based algorithm development, QDK’s optimizing compilers, and its suite of high-performance simulators—including sparse state-vector, full state-vector, and resource estimation backends. The Qiskit [34] plugin provides an alternative pathway with circuit construction, transpilation, and execution capabilities targeting other Qiskit-compatible backends. Users can choose whichever ecosystem best suits their needs, and the uniform QDK/Chemistry interface ensures that workflow logic remains unchanged regardless of backend selection, allowing the path from prototyping to hardware execution without workflow modifications.

4 Conclusions

QDK/Chemistry provides infrastructure for quantum chemistry workflows that bridges classical electronic structure and quantum algorithm design. Beyond delivering high-performance software components, the toolkit’s architecture enables diverse methods to interoperate within a unified framework by separating data from algorithms, exposing factory-based interfaces, and supporting plugins for external packages.

This design serves the varied needs of the quantum chemistry community. Method developers can contribute new algorithms at any workflow stage while relying on validated implementations elsewhere. Application scientists can systematically compare approaches by swapping components through factory interfaces rather than rewriting pipeline logic. As quantum hardware matures, individual workflow stages can evolve independently—incorporating new methods, hardware interfaces, or error mitigation strategies—without disrupting established workflows. Serialization support for all intermediate artifacts provides the provenance tracking essential for reproducible science.

We view QDK/Chemistry as a foundation for community development. The source code is available at <https://github.com/microsoft/qdk-chemistry>, and the package can be installed via `pip install qdk-chemistry` from PyPI.² Researchers can develop and distribute extensions independently, without requiring changes to the core codebase or coordination with other contributors. By reducing the friction of building, sharing, and comparing quantum chemistry workflows, we aim to accelerate progress in understanding which classical and quantum methods best address the electronic structure problems that motivate this field.

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A Example workflow code

This appendix provides a complete example demonstrating a typical QDK/Chemistry workflow, from molecular geometry specification through quantum phase estimation. The example illustrates the modular design principles discussed in Section 2, showing how different workflow stages compose through uniform interfaces.

Listing : Complete QDK/Chemistry workflow example.

```
1 # QDK/Chemistry end-to-end example
2 # Ground state energy estimation via Quantum Phase Estimation
3
4 import numpy as np
5 from qdk_chemistry import algorithms as algo
6 from qdk_chemistry.data import SciWavefunctionContainer, Structure,
    Wavefunction
7 from qdk_chemistry.utils import compute_valence_space_parameters
8
9 # Import plugins for backends
10 import qdk_chemistry.plugins.qiskit
11 import qdk_chemistry.plugins.pyscf
12
13 # -----
14 # Step 1: Define molecular structure
15 # -----
16
17 # Structure: common representation for all algorithms
18 # Create stretched H2 molecule
19 structure = Structure(
20     np.array([[0, 0, 0], [0, 0, 2.5]]),
21     symbols=["H", "H"]
22 )
23
24 # -----
25 # Step 2: Self-Consistent Field (SCF) calculation
26 # -----
27
28 # Factory pattern: algo.create(category, [method])
29 # Common interface: run(input, **params) -> output
30 # Using the PySCF SCF backend; alternatives include "qdk"
31 scf_solver = algo.create("scf_solver", "pyscf")
32 scf_energy, scf_wfn = scf_solver.run(
33     structure,
34     charge=0,
35     spin_multiplicity=1,
36     basis_or_guess="sto-3g"
37 )
38
39 # -----
40 # Step 3: Valence space selection
41 # -----
42
43 num_val_e, num_val_o = compute_valence_space_parameters(scf_wfn, charge=0)
44 valence_selector = algo.create(
45     "active_space_selector", "qdk_valence",
46     num_active_electrons=num_val_e,
47     num_active_orbitals=num_val_o
48 )
49 valence_wfn = valence_selector.run(scf_wfn)
50
51 # -----
```

```

52 # Step 4: Hamiltonian construction
53 # -----
54
55 ham_constructor = algo.create("hamiltonian_constructor")
56 active_hamiltonian = ham_constructor.run(valence_wfn.get_orbitals())
57
58 # -----
59 # Step 5: Qubit Hamiltonian (Jordan-Wigner encoding)
60 # -----
61
62 # Transform fermionic Hamiltonian to Pauli operators
63 # This example uses the Qiskit qubit mapper with Jordan-Wigner encoding
64 qubit_mapper = algo.create(
65     "qubit_mapper", "qiskit", encoding="jordan-wigner"
66 )
67 qubit_hamiltonian = qubit_mapper.run(active_hamiltonian)
68
69 # -----
70 # Step 6: Iterative Quantum Phase Estimation
71 # -----
72
73 # Run CASCI to get multi-configuration wavefunction
74 n_alpha, n_beta = valence_wfn.get_active_num_electrons()
75 casci = algo.create("multi_configuration_calculator", "macis_cas")
76 casci_energy, casci_wfn = casci.run(active_hamiltonian, n_alpha, n_beta)
77
78 # Prepare trial state from top 2 determinants (truncated and renormalized)
79 trial_wfn = casci_wfn.truncate(max_determinants=2)
80
81 # Generate sparse state prep circuit (GF2 + X method)
82 state_prep = algo.create("state_prep", "sparse_isometry_gf2x")
83 state_prep_circuit = state_prep.run(trial_wfn)
84
85 # Create and configure IQPE
86 iqpe = algo.create(
87     "phase_estimation",
88     "iterative",
89     num_bits=8,           # Number of phase bits
90     evolution_time=0.5   # Evolution time
91 )
92
93 # Build the time evolution unitary via Trotter decomposition
94 evolution_builder = algo.create("time_evolution_builder", "trotter")
95
96 # Map controlled time evolution into circuit via Pauli sequence mapper
97 circuit_mapper = algo.create(
98     "controlled_evolution_circuit_mapper",
99     "pauli_sequence"
100 )
101
102 # Use QDK full state simulator to execute circuit and collect bitstrings
103 circuit_executor = algo.create("circuit_executor", "qdk_full_state_simulator")
104
105 # Run IQPE with the configured inputs
106 result = iqpe.run(
107     state_preparation=state_prep_circuit,
108     qubit_hamiltonian=qubit_hamiltonian,
109     circuit_executor=circuit_executor,
110     evolution_builder=evolution_builder,
111     circuit_mapper=circuit_mapper,
112 )
113
114 # Extract energy from phase estimation result
115 qpe_energy = result.raw_energy
116
117 print("QPE Results (10-bit precision):")

```

```
118 print(f"Reference CASCI energy: {cascl_energy:.6f} Ha")
119 print(f"QPE total energy: {qpe_energy:.6f} Ha")
120 print(f"Diff from CASCI: {abs(qpe_energy - casci_energy):.3e} Ha")
```

B Acronyms

ABI application binary interface

API application programming interface

ASCI adaptive sampling configuration interaction

AVAS atomic valence active space

CAS complete active space

CASCI complete active space configuration interaction

DFT density functional theory

FCI full configuration interaction

HF Hartree-Fock

MACIS Many-body Adaptive Configuration Interaction Solver

MC multi-configuration

MCSCF multi-configuration self-consistent field

MP2 second-order Møller-Plesset perturbation theory

QDK Quantum Development Kit

QPE quantum phase estimation

SCF self-consistent field

VQE variational quantum eigensolver